

Se-(8-Azidoadenosyl)selenomethionine

135608-83-2 | DTXSID70159478

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 5.16e-01

Global applicability domain: Outside

Local applicability domain index: 1.38e-01

Confidence level: 7.00e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>N,N,N',N',N'',N''-Hexakis(methoxymethyl)-1,3,5-triazine-2,4,6-triamine</div> <div>Measured: 0.54</div> <div>Predicted: 6.53e-01</div>	<div>Image not found</div> <div>Docusate sodium</div> <div>Measured: 0.97</div> <div>Predicted: 9.52e-01</div>	<div>Image not found</div> <div>Tris(2-butoxyethyl)phosphate</div> <div>Measured: 0.76</div> <div>Predicted: 8.01e-01</div>
<div>Image not found</div> <div>Tris(2-hydroxyethyl)isocyanurate</div> <div>Measured: 0.2</div> <div>Predicted: 2.08e-01</div>	<div>Image not found</div> <div>Malaoxon</div> <div>Measured: 0.05</div> <div>Predicted: 1.75e-01</div>	